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Effect of crystal-field split-off hole and heavy-hole bands crossover on gain characteristics of high Al-content AlGaN quantum well lasers

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The optical gain characteristics of high Al-content AlGaN quantum wells (QWs) are analyzed for deep UV lasers. The effect of crystal-field split-off hole (CH) and heavy-hole (HH) bands crossover on the gain characteristics of AlGaN QW with AlN barriers is analyzed. Attributing to the strong transition between conduction–CH bands, the TM spontaneous emission recombination rate is enhanced significantly for high Al-content AlGaN QWs. Large TM-polarized material gain is shown as achievable for high Al-content AlGaN QWs, which indicates the feasibility of TM lasing for lasers emitting at $\sim$220–230 nm. © *2010 American Institute of Physics*. [doi:10.1063/1.3488825]

Visible III-nitride lasers and light-emitting diodes (LEDs) are important for medical, storage, and illumination applications.[1–13] In contrast to visible nitride LEDs,[1–13] advances have only been realized for deep UV LEDs recently.[14–22] The applications of deep UV lasers cover free space communication and biochemical agent detection. The pursuit of AlGaN deep UV lasers is still challenging[23–29] due to (1) growth challenges of high Al-content AlGaN and (2) lack of understanding in gain characteristics of the quantum well (QW) employed for deep UV laser. Recent works have been reported for low[26–29] and high[23,30,31] Al-contents AlGaN QWs. However, these works were focused on the quantum efficiency of AlGaN QWs LEDs.[14–22,26–29] The pursuit of electrically injected AlGaN QWs lasers have been limited to emission wavelength (λ) $\sim$320–360 nm,[26–28] while only optically pumped deep UV laser had been realized.[23]

Recent theoretical studies have been carried out for analyzing the optical properties of both low Al-content[32–34] and high Al-content AlGaN QWs.[35] The studies on the gain characteristics for high Al-content AlGaN QWs are still relatively lacking. The improved understanding in the physics of optical gain of high Al-content AlGaN QW is important in identifying the limitations and potential solutions for achieving low-threshold and high-efficiency lasers in the deep UV spectral regime ($\lambda \sim$220–300 nm).

In this work, the gain characteristics and polarization properties of high Al-content AlGaN QWs active region are calculated and analyzed. The characteristics of the gain and spontaneous emission rate of high Al-content AlGaN QWs are compared with those of low Al-content AlGaN QWs. The crossover of crystal-field split-off hole (CH) and heavy hole (HH)/light-hole (LH) bands for high Al-content AlGaN QWs is found to have significant impact on the gain properties for deep UV active regions.

The optical gain and spontaneous emission properties of the compressively strained $Al_xGa_{1-x}N$ QW with AlN barriers are analyzed. The calculations of the band structures and wave functions for AlGaN QWs were carried out by using self-consistent six-band $\boldsymbol{k}\cdot\boldsymbol{p}$ formalism for wurtzite semiconductor taking into account the valence band mixing, strain effect, polarization fields, and carrier screening effect.[36–39] The band parameters for the III-nitride alloys utilized in our calculations were obtained from Refs. 39–41.

The valence band-edge energy levels (HH, LH, and CH) for $Al_xGa_{1-x}N$ as a function of Al-content (x) are shown in Fig. 1. For $Al_xGa_{1-x}N$ with $x<57.2\%$, the band-edge energy levels for HH and LH bands are larger than that of the CH band. The band-edge energy separations between HH/LH bands and CH band reduce with increasing Al-content, and the HH/LH and CH bands have a crossover at $x=57.2\%$. For $Al_xGa_{1-x}N$ with $x>57.2\%$, the band-edge energy level of CH band becomes larger than those of HH/LH bands, and this energy separation further increases as the Al-content in AlGaN alloy increases. The HH and CH bands crossover is important, as the transition between conduction and CH bands is transverse magnetic (TM)-polarized component.

Figure 2(a) shows the spontaneous emission recombination rate per unit volume (R_{sp}) for 3 nm $Al_xGa_{1-x}N$ QW ($x=20\%-80\%$) sandwiched by AlN barrier layers with carrier density (n) of 3×10^{19} cm^{-3} at T=300 K. The spontaneous emission rates (R_{sp}) for low Al-content AlGaN QW show dominant transverse-electric (TE) polarization, which is an order of magnitude higher in comparison to that for the TM polarization. Both the TE- and TM-polarized R_{sp} show increasing trend for increasing Al-content, which are attributed primarily to the larger momentum matrix elements for higher Al-content AlGaN QWs. The TM-polarized R_{sp} starts to exhibit large increase for $x>\sim58\%$. For $Al_xGa_{1-x}N$ QW with $x\sim68\%$, both TE- and TM-polarized components are similar. For high Al-content above 68%, the TM-polarized R_{sp} is

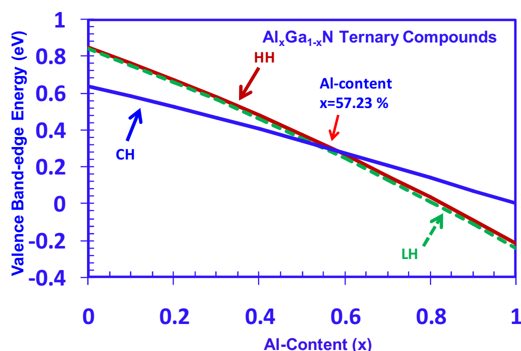

FIG. 1. (Color online) Energy band edges of the HH, LH, and CH bands as a function of Al-content (x) for $Al_xGa_{1-x}N$ ternary compounds.

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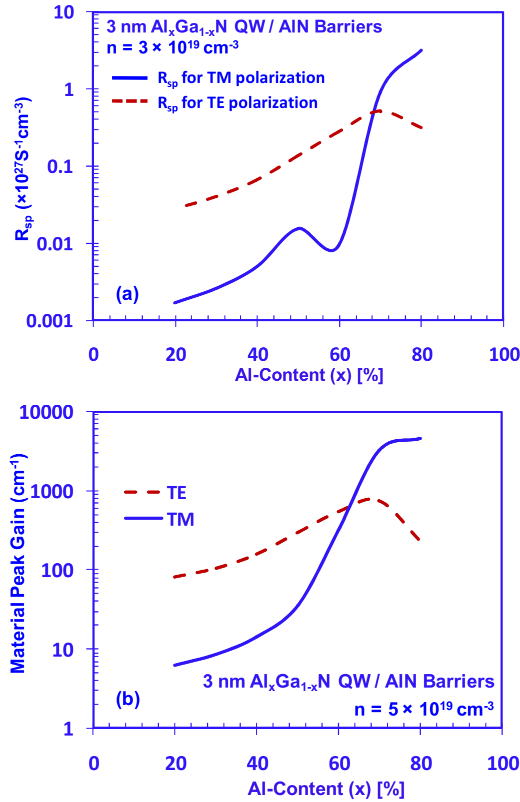

FIG. 2. (Color online) TE- and TM-polarized (a) spontaneous emission rate (R_{sp}) and (b) peak material gain for 3 nm thick $Al_xGa_{1-x}N$ QWs with AlN barriers as a function of different Al-contents (x).

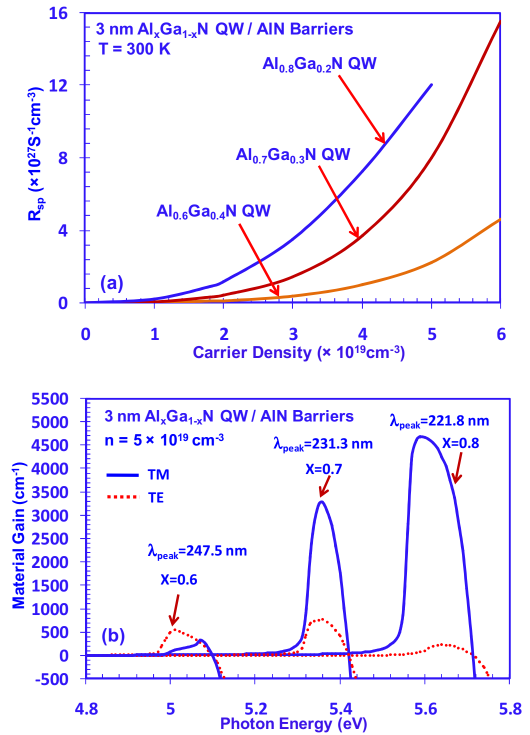

FIG. 3. (Color online) (a) Spontaneous emission radiative recombination rate (R_{sp}) as a function of carrier density, and (b) TE-polarized and TM-polarized optical gain spectra for 3 nm $Al_xGa_{1-x}N$ QWs with AlN barriers with x=60%, 70%, and 80%.

significantly enhanced attributing to the strong transition between conduction band and CH band. The reduction in the TE-polarized R_{sp} for high Al-content AlGaN QW can be attributed to the significantly lower carrier density populating the HH and LH bands from the increasing energy separation between CH and HH/LH bands.

Figure 2(b) shows both the TE (g_{peak}^{TE}) and TM peak material gains (g_{peak}^{TM}) as a function of Al-content for the 3 nm $Al_xGa_{1-x}N$ QW with AlN barriers calculated for $n=5\times10^{19}$ cm^{-3} at T=300 K. For $Al_xGa_{1-x}N$ QW with $x<68\%$, both the g_{peak}^{TE} and g_{peak}^{TM} are relatively low (g_{peak} <500 cm^{-1}), however the g_{peak}^{TE} is relatively larger than the g_{peak}^{TM}. For $Al_xGa_{1-x}N$ QW with $x>68\%$, the g_{peak}^{TM} is dominant resulting in significantly higher peak gain (g_{peak}^{TM} =3280 cm^{-1} for x=70%, and g_{peak}^{TM}=4690 cm^{-1} for x=80%). The gain analysis indicates that the carriers in the high Al-content AlGaN QW are dominantly confined in the CH band after the crossover of the HH/LH and CH bands, resulting in higher than one-order of magnitude ratio of $g_{peak}^{TM}/g_{peak}^{TE}$ ratio.

Figure 3(a) illustrates the spontaneous emission recombination rate per unit volume (R_{sp}) for 3 nm thick $Al_xGa_{1-x}N$ QW sandwiched by AlN barrier layers with carrier density (n) up to $n=6\times10^{19}$ cm^{-3}. The analysis was carried out for AlGaN QW with x=60%–80%. For the $Al_{0.7}Ga_{0.3}N$ QW (or $Al_{0.8}Ga_{0.2}N$ QW), the increase in the spontaneous emission rate (R_{sp}) as a function of carrier density ranges between 3.4–3.9 times (or 5.4–10.5 times) higher compared to that of the $Al_{0.6}Ga_{0.4}N$ QW. The enhancements of the R_{sp} for high Al-content (x=70%,80%) AlGaN QWs are attributed to the increase in the TM-polarized spontaneous emission rate for AlGaN QW with Al-content above ~68%.

Figure 3(b) shows the TE- and TM-polarized optical gain spectra for $Al_xGa_{1-x}N$ QWs with x=60%–80%. The peak gain wavelengths (λ_{peak}) for $Al_xGa_{1-x}N$ QW with x=60%, 70%, and 80% are 247.5 nm, 231.3 nm, and 221.8 nm, respectively. For $Al_{0.6}Ga_{0.4}N$ QW, both the TE- and TM-polarized gains are relatively low (~400–500 cm^{-1}). However, for the case of higher Al-contents (x=70%, x=80%), the TM-polarized gains increase dramatically, while the TE-polarized gains are significantly lower.

Figures 4(a) and 4(b) show the TM- and TE-polarized material gains (g_{peak}^{TM} and g_{peak}^{TE}) for high Al-content AlGaN QW as a function of carrier density, respectively. The g_{peak}^{TM} for the $Al_{0.7}Ga_{0.3}N$ QW and $Al_{0.8}Ga_{0.2}N$ QW are found to be significantly larger. For $Al_{0.7}Ga_{0.3}N$ QW, the g_{peak}^{TM} is 1.5–4.3 times larger than that of the g_{peak}^{TE}. For $Al_{0.8}Ga_{0.2}N$ QW, the g_{peak}^{TM} is ~20–110 times than that of the g_{peak}^{TE}, attributing to its significantly larger energy separation of the CH and HH/LH bands. At $n=5\times10^{19}$ cm^{-3}, the g_{peak}^{TM} of $Al_{0.8}Ga_{0.2}N$ QW and $Al_{0.7}Ga_{0.3}N$ QW are 4690 cm^{-1} and 3280 cm^{-1}, respectively. The g_{peak}^{TE} of $Al_{0.8}Ga_{0.2}N$ QW and $Al_{0.7}Ga_{0.3}N$ QW were found as 230 cm^{-1} and 765 cm^{-1} (at $n=5\times10^{19}$ cm^{-3}), which are relatively negligible compared to the g_{peak}^{TM}. In contrast to the higher Al-content AlGaN QWs, the g_{peak}^{TE} and g_{peak}^{TM} are relatively similar for the $Al_{0.6}Ga_{0.4}N$ QW. The g_{peak}^{TE} and g_{peak}^{TM} of the $Al_{0.6}Ga_{0.4}N$ QW at $n=7\times10^{19}$ cm^{-3} are 1425 cm^{-1} and 1610 cm^{-1}, respectively. Thus, the TM-polarized lasing is feasible for high Al-content AlGaN QW lasers in the 220–230 nm spectral range.

To analyze the threshold properties of deep UV lasers, AlGaN QW lasers with optical confinement factor (Γ_{opt}) of 0.02 (Ref. 33) were employed in the analysis. The internal losses (α_i) in typical AlGaN lasers range from 14 cm^{-1} (Ref.

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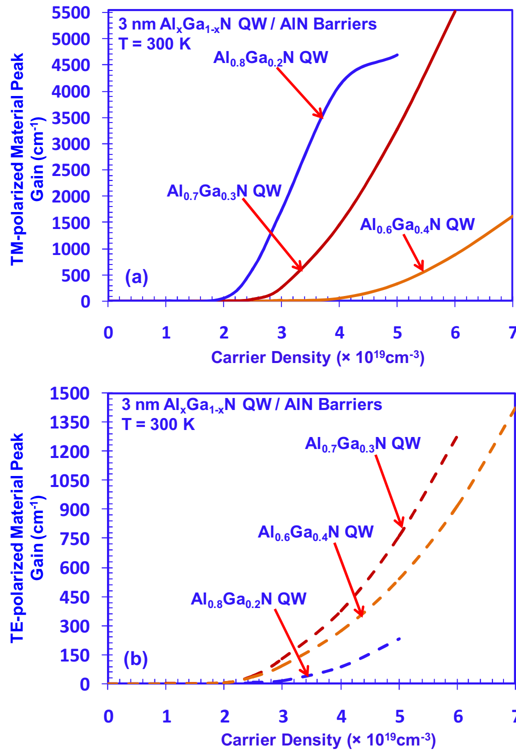

FIG. 4. (Color online) (a) TM-polarized material gain (g_{peak}^{TM}) and (b) TE-polarized material gain (g_{peak}^{TE}) as a function of carrier density for 3 nm thick $Al_xGa_{1-x}N$ QWs with AlN barriers with x=60%, 70%, and 80%.

27) up to 50 cm^{-1}.[33] The laser cavity length is assumed as 500 μm with end-facet reflectivities of 95% and 35%, which correspond to mirror loss (α_m) of 11 cm^{-1}. The threshold gains (g_{th}) are estimated as $\sim$1250 cm^{-1} (α_i=14 cm^{-1}) and $\sim$3050 cm^{-1} (α_i=50 cm^{-1}). For the lasers with g_{th} $\sim$1250 cm^{-1}, the threshold carrier densities (n_{th}) are 2.8×10^{19} cm^{-3} and 3.9×10^{19} cm^{-3} for $Al_{0.8}Ga_{0.2}N$ QW and $Al_{0.7}Ga_{0.3}N$ QW, respectively. For the lasers with g_{th} $\sim$3050 cm^{-1}, the threshold carrier densities (n_{th}) of 3.5×10^{19} cm^{-3} and 4.9×10^{19} cm^{-3} are obtained for $Al_{0.8}Ga_{0.2}N$ QW and $Al_{0.7}Ga_{0.3}N$ QW, respectively.

In summary, the gain characteristics of the high Al-content AlGaN QWs are analyzed for deep UV lasers. The effect of CH and HH bands crossover on the gain for the AlGaN QWs for lasers is clarified. After the crossover of the HH/LH and CH bands, the band-edge energy level of CH band is larger than those of the HH/LH bands. The TM-polarized R_{sp} and material gain are dominant for AlGaN QW with $x>68\%$. The spontaneous emission rate is significantly enhanced for high Al-content $Al_xGa_{1-x}N$ QW (x=70%, 80%) attributing to the strong transition between conduction band and CH band. The gain analysis shows that large TM-polarized material gain as achievable for high Al-content $Al_xGa_{1-x}N$ QWs, which indicates the feasibility of TM lasing for deep UV lasers emitting at $\sim$220–230 nm.

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